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Large supercrystals promise superior sensors

Improved sensitivity could improve security in public places

by Neal Singer

Using an artful combination of nanotechnology and basic chemistry, Sandia researchers have encouraged gold nanoparticles to self-assemble into unusually large supercrystals that could significantly improve the detection sensitivity for chemicals such as explosives or drugs.

“Our supercrystals have more sensing capability than regular spectroscopy instruments currently in use, just like a dog’s nose has more sensing capabilities than a human’s,” said lead Sandia researcher Hongyou Fan.

Other researchers previously reported forming gold supercrystals but only in the micron range, too small for commercial production, said Hongyou, whose submillimeter supercrystals are easily manipulable with industrial tools of the macroworld.

The benchtop sensors, recently reported in Nature Communications, also are surprisingly inexpensive, Hongyou says. “The supercrystals are built of gold, but only a little of it.” It takes 0.012 grams of gold to form a sensor, for a total materials cost of roughly 50 cents.

To form each of the Sandia supercrystals, millions of gold nanoparticles tightly self-assemble in orderly rows. The particles naturally develop facets — resembling those cut in diamonds by a jeweler — to exist at the lowest possible energy level needed to maintain the existence of the crystal.

Crystal facets ‘bay’ like hounds

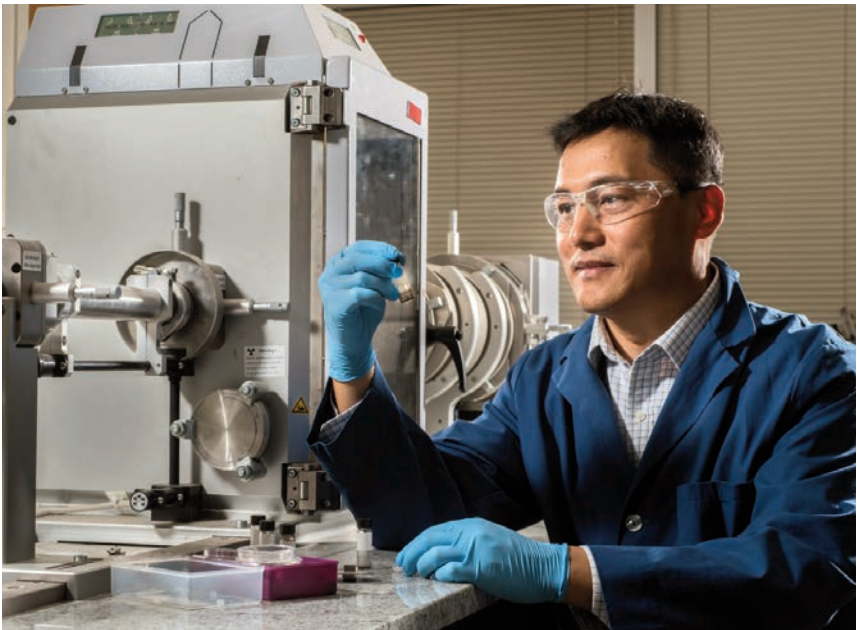
The facets are also adept at recognizing and transmitting signals. They “bay” in groups like hounds — that is, emit a strong signal — when a predetermined external frequency is “sniffed.” That is because when a

nanoparticle recognizes a band frequency and makes it resonate, that energy will pass to other nanoparticles, coupled by nearness and the local electro-magnetic field. The alerted nanoparticles augment the response in a kind of echoing action, making noticeable what in less keen sensors may have passed unnoticed.

The initial formation of the crystals involves dispersing gold particulates about 5 nanometers in diameter into a “good” solvent, toluene. They then are subjected to a bath in a “hostile” solvent, isopropanol, which the particles supersaturate and from which they are then ejected or precipitated.

The ejected particles, refugees from the solution, then crystallize as small seeds. The growth of facets makes them available to respond to a wide variety of incoming chemical odors or light band frequencies.

The proper concentrations of materials and particle immersion times are important factors in creating large



GOLDEN AND SUPER TOO — Sandia researcher Hongyou Fan holds a vial of gold supercrystals he is preparing to characterize in a small-angle X-ray scattering instrument (the horizontal bar). Behind him is the large chamber in which his samples are placed during supercrystal experiments. (Photo by Randy Montoya)

crystals. The process may take as long as a week.

The work was funded by the DOE’s Basic Energy Sciences office and by Sandia’s Laboratory Directed Research and Development program. Work was carried out in part at the Center for Integrated Nanotechnologies, a DOE Office of Science user facility jointly managed by Sandia and Los Alamos national laboratories.

Progress toward plugging an antibiotic pump

Sandia computer modeling reveals pump mechanism and essential ‘lock’



RESISTANCE CAN BE DEADLY — Susan Rempe stands in front of the Center for Integrated Nanotechnologies, where some of her research on bacterial pumps was done. Her team from Sandia and the University of Illinois at Urbana-Champaign are studying the pumps to understand the mechanisms behind antibiotic resistance in bacteria. (Photo by Randy Montoya)

By Mollie Rappe

Each year in the U.S., at least 23,000 people die from infections caused by antibiotic resistant bacteria, according to the Centers for Disease Control and Prevention.

Using computer modeling, researchers from Sandia and the University of Illinois at Urbana-Champaign are helping to develop the means to prevent some of those deaths.

One way bacteria develop resistance to many different antibiotics is by producing pumps that spit out unfamiliar small molecules, such as antibiotics, before they can do any damage. The researchers teased out the details of how one antibiotic pump works.

The eventual goal is to develop new drugs to plug the pump so it cannot spit out antibiotics, perhaps restoring their effectiveness, said Susan Rempe, Sandia computational biophysicist. She added, “Now that we have the structure of the pump and know how it works, scientists can design a molecule that sticks tightly to the transporter. I think that’s doable in the near-term, maybe five years.”

The research was published recently in the Proceedings of the National Academy of Sciences.

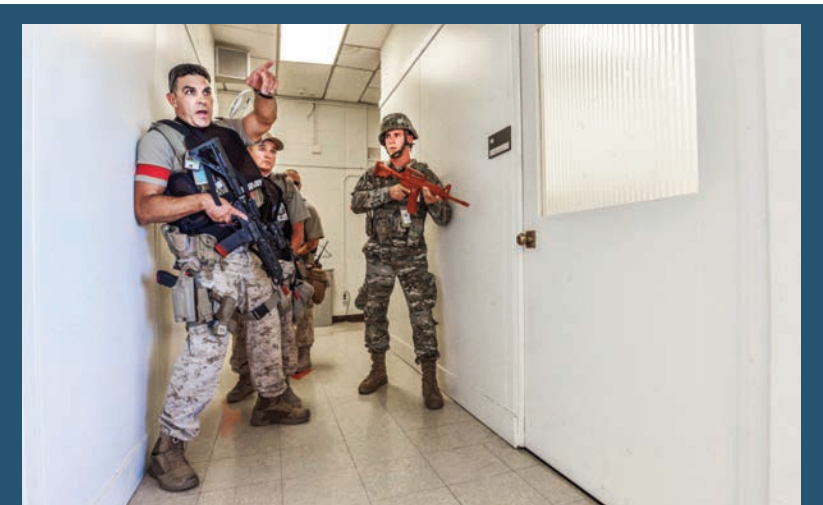
Refining data to determine pump’s detailed structure

The specific pump researchers studied, called EmrE, comes from E. coli, common bacteria that occasionally cause food poisoning. The pump recognizes and removes moderately oily, positively charged small molecules, said Josh Vermaas, a former Illinois graduate student whose work with Susan was supported through Sandia’s Campus Executive Program. Many common antibiotics, including streptomycin, doxycycline and chloramphenicol, are oily and positively charged.

Their first step was to determine a detailed structure of the pump. The starting structure of the pump was very rough, missing many of the essential chemical details, and misshapen, Vermaas said. Susan added it can be particularly challenging to get good structural data of drug transporters like EmrE because they are flexible. Imagine having to take a picture of a wriggling toddler with a sluggish camera: the resulting photo is more of a blur than an exact likeness.

They combined experimental data from a variety of common biophysical methods such as X-ray crystallography, cryo-electron microscopy and electron paramagnetic resonance spectroscopy, as well as decades of knowledge of the most likely internal arrangements of amino acids, the building blocks of proteins, to produce a high-resolution structure of the pump.

(Continued on page 6)



“THEY’RE INSIDE” — Security forces from Sandia and the 377th Air Base Wing at Kirtland prepare to stop a mock shooting incident during the Labs’ July 25 Annual Exercise. See more photos by Randy Montoya on page 8.

20 years of atmospheric science in the Arctic celebrated at barbecue

By Neal Singer

A community barbecue featuring science talks, door prizes and even boat races celebrated 20 years of research on the changing Arctic climate in mid-July for the Sandia-managed Atmospheric Radiation Measurement center in Utquagvik (formerly Barrow), Alaska.

An overflow local crowd learned how scientists have used ARM’s capabilities to deploy airplanes, ships, balloons and most recently drones to gather extensive data on Arctic atmospheric conditions and processes. Phenomena studied include cloud formation, atmospheric ice formation, radiation — blocked, reflected or absorbed — snow and rainfall, wind conditions and changes at various levels of the oceans’ shallow and deep currents.

Door prizes provided by private donors were geared for an intrepid crowd: a GPS device, a camping solar-panel charger, a Coleman stove, a thermos, an LED headlamp and a quadcopter drone, so-called due to its four propellers.

“We worked with our colleagues at the Alaska native corporation UIC Science (Ukpeaġvik Iñupiat Corp) on the event,” said Mark Ivey, Sandia manager of the ARM site. “A terrific fellow named Kaare Erickson from UIC cooked hamburgers and hotdogs — not whale meat, sorry.”

Arctic amplifies climate changes

Interest continues in northernmost North America because, explained Bernie Zak, retired Sandia researcher and ARM’s initial manager, “Changes in climate are amplified in the Arctic.”

Bernie, who was tapped by current site manager Mark Ivey to be a featured speaker at the celebration, said there’s a dramatic difference in Earth’s heat absorption when ice and snow, which reflect heat, melt and vanish. Only water and earth — both good heat absorbers — remain to take their place.

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Lab News Notes

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Also soot, which flies all over the world as fine particles, or aerosols, has a larger heat-absorption effect when it lands on the Arctic’s white snow and ice than on the already dark earth and water of the lower latitudes. “In the Arctic, it’s a magnified effect: as the level of snow melts, the recent soot gets added to the old soot below it, and the surface gets darker and darker,” he said.

Bernie is credited with helping to give birth to and then guide the Alaskan ARM facility in Utquagvik — the most northern of several ARM sites funded by DOE — over its first decade.



SKIN BOAT RACE — Four native crews, in four seal-skin boats used in the community’s spring whale hunt, prepare to race for a prize of gasoline. Usually held on July 4, the race was postponed due to bad weather and rescheduled so it would be part of the festivities at the Atmospheric Radiation Measurement center barbecue. The boats launched, raced across the central lagoon in Barrow, Alaska, touched an observer on the far side, then rowed back. First boat to land at the launch point won. (Photo by Mark Ivey)

Bernie graduated first in his class in physics in 1963 from DePaul University in Chicago and earned a doctorate in the same subject from the University of California, Berkeley in 1971. His climate research path began after a three-year stint at Lawrence Berkeley National Laboratory, when he came to Sandia to work with hazardous aerosols and air pollution. In the 1980s, his focus migrated slightly to study the concept of nuclear winter, which postulated that “if there were ever a global nuclear war, there would be so much dust and smoke launched into the atmosphere, there’d be no summer for maybe two or three years,” Bernie said.

National security interests

In that case, he continued, “the northern hemisphere would lose more population from starvation than from the weapons. So, the condition was of interest to Sandia as a national security threat.”

From there, “it was a relatively easy transition into the climate program,” he said, and when DOE solicited applications in 1991 for people to head up the three ARM sites, he was chosen to head the northern site.

But before work began, “there was a hiatus,” he said. “There was no funding to proceed.”

That situation changed in 1996 when the DOE provided funds to proceed with the development and operation of what became the DOE North Slope of Alaska ARM facility. This coincided with the National Science Foundation’s initiation of the Surface Heat Budget of the Arctic project, which was joined by multiple agencies and universities. SHEBA involved the year-long drift of an instrumented icebreaker rented from the Canadian government and intentionally frozen into the Arctic ice pack.

Thinning ice pack

“The intent was to freeze the ship into ice a meter thick, but it had been decades since anyone took a serious look at the Arctic ice pack,” said Bernie. “It was hard to find ice a half-meter thick.” So study of the Arctic became “hot,” he said, “because we were observing changes long predicted in climate models.”

The icebreaker’s screw propellers were turned off, but the ship remained powered for heat and light. Scientists flew in and out by helicopter, working to determine the condition of the ocean at various levels as well as wind and other atmospheric phenomena.

“So we received funding from DOE to implement the Alaskan ARM program, and we established the research station at Utquagvik as a support site,” Bernie said. “It wasn’t planned as a pre-eminent facility, but that’s the

way it’s been working out. It allowed us to observe changes that provided data for our models to forecast future changes,” Bernie said.

Data supported projections

“It was gratifying that data coming in were supportive of projections that had been made of changes in the Arctic, although we were surprised at the rapidity with which this was taking place,” he added. “There was shrinkage of snow coverage; it disappeared earlier in spring and returned later in fall.”

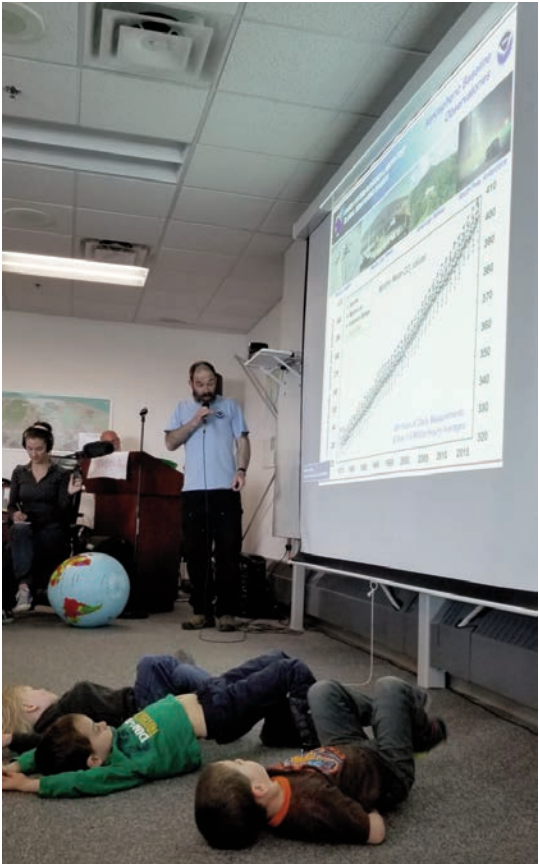
In addition to Bernie, presentations were made by Alistair Rogers of Brookhaven National Laboratory and Bryan Thomas from the National Oceanic and Atmospheric Administration and the Barrow Observatory.

“Hans Verlinde (of ARM and Penn State University) also gave a wonderful presentation about arctic clouds,” said Mark.

Mark, who took over management of the site for Sandia in 2010 when Bernie retired, honored Walter Brower, ARM facility site manager and Jimmy Ivanoff, ARM chief operator, both from UIC, along with Verlinde for almost 20 years of service to ARM, and they received warm applause from the crowd.

Mark said, “We were very glad for the big turnout and hope to do similar events in the future. I’d like to mention that without the support of the native community in Utquagvik, where we are guests, scientific work would not be possible. They have actually set aside a large tract of land for long-term environmental studies, and they are very interested in the outcomes of programs like ours.”

Upcoming is another icebreaker deployment for scientific observation, which Mark said is planned for next year as part of the NSF’s MOSAIC, or Multidisciplinary drifting Observatory for the Study of Arctic Climate, a multi-national, multi-agency campaign.



FUTURE DATA DIVAS — Taking in 40 years of atmospheric carbon dioxide measurements by scientists in Alaska, Hawaii and American Samoa are three local children awaiting the barbecue celebrating the 20th anniversary of DOE’s and Sandia’s Atmospheric Radiation Measurement center in Utquagvik, Alaska. Bryan Thomas of the National Oceanic and Atmospheric Administration presented the data. (Photo courtesy of Cheryl Humme)

Finding an inclusive vision for working parents

Parents group ups support of older, established families

By Troy Rummler

Employee groups grow up so fast. Before you know it, they become more mature, they develop new interests and passions and their names change. Now in its third year, the organization formerly known as the New and Expectant Parents Group is rapidly expanding its mission to support more diverse family situations and has changed its name to the Sandia Parents Group (SPG) to match its new identity.

“It’s more inclusive,” said Liza Kittinger, an SPG board member and systems analyst. “We wanted to focus on not just new and expectant parents but all parents going through any stage of parenthood.”

Among other changes, the group’s monthly luncheons, which in the past hosted discussions tailored to parents with babies, will cover a wider range of issues such as navigating school choice and adoption. The group also plans to include more California-based employees.

“In all of those stages you need support, resources and a trusted community you can depend on,” Liza said.

The group welcomes moms, dads and caregivers of children under the age of 18, regardless of race, sexual orientation or gender. The group continues to serve individuals planning for a biological, adopted or foster child, and those in nontraditional parenting roles, such as grandparents raising grandchildren.

Advocates for policy that retains parents

Co-founder Christina Beppler says she has seen talented colleagues leave the Labs to pursue job opportunities closer to family because they didn’t feel adequate support at work. That’s a problem, she says, because fulfilling Sandia’s mission “only happens when people stay here, they learn, become an expert in their area, then start passing that on to people who are coming in.”

With an eye on recruitment and retention, SPG has added a management engagement subcommittee that encourages executive leadership across the Labs to enact family-friendly policies and procedures.

“Our group is in support of any existing, new or changed policies that recruit, engage and retain working parents,” said Christina, an energetic materials scientist and a winner of the 2018 Albuquerque Moms Blog Mom of the Year award.

SPG meets regularly with Renee Holland, director of Employee Health Services, and shares information and feedback from its members with Renee and her team. SPG has helped human resources communicate benefits information more clearly and improve access to nursing mothers’ rooms.

“We are committed to supporting a healthy pregnancy and assisting the facilitation for new, expecting and all parents at Sandia to be happier and healthier role models for their children,” Renee said.



GONE FISHIN’ — The Sandia Parents Group organizes regular events in the community for parents and families, including this outing to the ABQ BioPark Aquarium. (Photo courtesy of the Sandia Parents Group)

The group also asked Cliff Renschler, director of the component science center, to champion the group among management.

“I readily agreed because I believe in what they are trying to do,” Cliff said.

He points to a survey Sandia Parents Group conducted to better understand the Labs’ demographics and the needs of parents. “The analysis of those survey results may point to unmet needs that would need executive management attention to address,” he said. “I hope to be able to provide some measure of value at that point.”

Building on a legacy

In February, Family Friendly New Mexico awarded Sandia gold recognition, its highest honor, for family-friendly policies. Christina says the award shows a legacy culture of supporting parents at the Labs, but she believes there’s a need to build on it. She and Liza say, for example, that some parents face criticism that they’re less focused than coworkers with fewer at-home responsibilities. This could make them unwilling to speak up when they have needs related to taking care of their kids.

“We can make Sandia a place people are excited to bring their whole selves, including their families,” says Catherine Siefert, an SPG event organizer and mechanical engineer.

Sandia Parents Group has been collaborating the Sandia Women’s Action Network and other employee resources groups.

“More moms are in the workforce than ever before, either by choice or because they have to be,” Liza said. “Balancing motherhood and a full-time career can have challenges. SWAN fully understands how to advance women in the workforce, which makes them a great partner.”

Another shared goal is improving access to information about policies and benefits. When Christina was getting ready to have a child, she didn’t know what to do or whom to talk to about benefits. Now, she’s making sure SPG is a one-stop shop for up-to-date information.

“If you come talk to us, we’re going to get you in touch with the right person today. You won’t have to search for it.”

Visit parents.sandia.gov or email Christina at clcrawf@sandia.gov for resources, upcoming events and ways to get involved with the group.

Sandia researchers named Combustion Institute fellows

by Michael Padilla

Sandia researchers Robert Barlow and Jacqueline Chen are among 125 members who have been named inaugural fellows of The Combustion Institute.

As dedicated members of the international combustion community, fellows are recognized by their peers as distinguished for outstanding contributions to combustion research, whether in combustion fundamentals or in applications. Fellows are active participants in the institute, as evidenced by the publishing of papers in the institute’s affiliated journals, attendance at the International Symposia on Combustion and attendance at the institute’s section meetings.

Robert was recognized for development and application of optical diagnostics for scalar measurements in turbulent flames, providing insights into turbulence-chemistry interactions, according to the institute. Robert’s work has focused on the simultaneous application of several lasers to instantaneously measure the chemical composition and temperature of partially burned gases in flames.

Jackie was recognized for direct numerical simulations elucidating the fundamental processes in turbulent flames in different modes of combustion, according to the institute.



Robert Barlow (Photo by Randy Wong)

Direct numerical simulation refers to a computationally costly but fully resolved type of simulation that resolves all turbulence and flame scales for a given chemical mechanism and therefore does not require model approximations to describe turbulence-chemistry interactions.

As researchers at Sandia’s Combustion Research Facility,

Robert and Jackie have expanded the fundamental knowledge of combustion processes while helping to advance cleaner, more efficient burners and engines.

“I am extremely proud of the accomplishments of Robert and Jackie,” said Bob Hwang, director of the Chemistry, Combustion, and Materials Center. “Being named as part of the inaugural class of fellows of The Combustion Institute is a testament to their hard work and commitment to Sandia. They represent the best in our outstanding combustion research community.”

The Combustion Institute is an international, non-profit educational and scientific society. Founded in 1954, the institute promotes and disseminates research activities in all areas of combustion science and technology for the advancement of many diverse communities around the world.

Robert Barlow, leader in turbulent combustion

Robert leads an experimental facility for measuring temperature and chemicals in flames, with a variety of lasers and diagnostic techniques being applied simultaneously to gain better understanding of complex interactions of turbulent mixing, molecular diffusion and chemical kinetics.

As a proponent of international collaboration in basic research, he has hosted numerous visiting students and combustion scientists.

Since 1996, Robert has served as the lead organizer of the International Workshop on Measurement and Computation of Turbulent Flames. The workshop provides a framework for accelerating the development of predictive, science-based numerical models that can aid in the design of advanced combustion systems with high efficiency and low emissions.

Jackie Chen, leader in direct numerical simulation

Jackie focuses her work on computational simulation of turbulent reacting flows with complex chemistry. She and her team have developed a state-of-the-art,

direct numerical simulation code called S3D. The code is the leading one of its kind for combustion applications and is used by combustion researchers and computer scientists worldwide.

Jackie has gleaned insights into fundamental turbulence-chemistry interactions underlying combustion in internal combustion engines, gas turbines and for high-speed propulsion. The simulation’s benchmarks created on the world’s fastest supercomputers also are used by the broader modeling community to develop and assess combustion and mixing models to develop efficient and clean engines operating on hydrocarbon and bio-derived fuels.

Jackie’s impact on fundamental turbulent combustion science underlying engines and especially on the computational members of The Combustion Institute has been expanded by the sharing of computational data for model validation and development. As a director of The Combustion Institute since 2007, she has served on numerous committees.

Also named fellows were former Sandia staff members James Miller, Stephen Klippenstein, Robert Kee, Simone Hochgreb, Mitchell Smooke and Reginald Mitchell; retired Sandia staff member and manager Donald Hardesty; and former Sandia postdoctoral appointees Evatt Hawkes, who worked with Jackie, and Fei Qi.

The complete list of fellows is available on The Combustion Institute’s website.



Jackie Chen (Photo by Randy Wong)

New Facilities system aims for one-stop, consistent space use



CENTER OF THE ACTION (Tech Area I) — Due to its large size and wide variety of mission requirements and security and ES&H concerns, facilities work in Tech Area I will be managed by Kimberly Pino and Rico Ortiz. (Photo by Norman Johnson)

Space: It's about a place you want to be

By Manette Newbold Fisher

As Sandia leadership looks toward fulfilling the Labs' operating principle of one lab, one system, a new vision for space management is taking hold.

For years, space was managed by 11 divisions in a decentralized model, leading to a constrained and unbalanced system, said Jack Mizner, centralized space manager. Space coordination generally was assigned to members of center support teams as a part-time focus. This, among other issues, led to inconsistency, space conflicts, short-term planning and lack of communication between divisions.

In June 2017, representatives from Facilities, Human Resources, Business Operations, Space and Asset Management and Information Technology began meeting to plan for the implementation of centralized space management.

The primary objective was a model based on organizational change management principles, project management tools and best practices. Jack and his team of strategic and tactical space planners continue to consult with division and center leadership to fine tune the new model.

Other sites benchmarked

Benchmarking studies of other space management approaches were conducted to inform Sandia's model, which included other Department of Energy sites (Los Alamos and Lawrence Livermore national laboratories and the Nevada National Security Site) and universities.

"This model is not new. While it's new to Sandia, companies do this all over the country and all over the world," Jack said. "They have professionals who work in this field."

Some of the most notable research the team gathered came from the University of Michigan's Space Utilization Initiative, which put into place space policies that are used across campus in a centralized space management approach, according to strategic space planner Jeff Smith. In doing so, the university avoided \$462 million in one-time capital costs and some \$18 million in estimated recurring operating costs.

Of particular interest to Sandia was a shift in Michigan's campus culture, where space is now considered an institutional

resource that must be shared and managed effectively for the good of the institution.

"In light of the short-term projected mission growth, space management is one of the only timely tools we have to help out — all the more important that this initiative is successful," said Lynne Schluter, Facilities director.

A new Sandia system

The new space management workflow begins with a need, Jack said, and the sooner the facilities organizations in New Mexico and California know about that need, the sooner the team of tactical space planners can help. Requests are submitted through the MAXIMO system, available on Techweb.

The space planners will work with centers and divisions, as well as HR, to make appropriate space assignments and coordinate any needed space modifications. Under the new model, key roles include:

- Strategic site planners interact with assigned divisions to understand needs and future Labs capabilities. They ensure Sandia addresses facilities and infrastructure requirements.
- Tactical space planners are responsible for the short-term management of space and will maintain data and metrics to inform longer-term decisions.
- Building managers will work with other team members to meet customer space needs and ensure work-spaces are safe and secure.
- Moves personnel ensure relocation needs are met, both for computing and physical/personal assets.

Together, the team will identify opportunities where space utilization can be improved.

Jack said the goal of the new space management structure is to ensure each division has appropriate and suitable space available for each member of Sandia's workforce and that the policy is consistently applied across Sandia. He also said the system aims to retain, attract and engage top talent at the Labs.

For more information on Centralized Space Management, including presentations, FAQ and contact information, employees can visit spacesolutions.sandia.gov.



CUSTOMER FOCUSED — Acting as a single point of contact for facilities needs in Tech Area V, Mark Coffing (right) coordinates with mission partners like Matt Burger, senior manager of for Nuclear Facilities and Applied Technologies. (Photo by Vince Gasparich)

Information technology upgrades key to Facilities overhaul

By Steve Scott

In preparing to overhaul the way the Infrastructure Operations Division works with its Facilities customers, Associate Labs Director John Clymo surveyed the course ahead and thought he saw an obstacle.

"I had the impression that IT support would be a hurdle to making these needed upgrades," he recalled. Instead, he says, the Facilities teams have come a long way largely because partners in Information Technology Services helped clear the path.

"I appreciate their commitment to supporting our vision," he said.

The Facilities overhaul involved major changes to processes for accepting and executing work, as well as a wholly revised system for cataloging and assigning work space across the Labs. IT teams made those changes easier, expanding two computer systems to meet the new needs and adding an array of new mobile services to streamline work.

First, software developers worked with Facilities team members to interview space planners, managers and other system users to thoroughly understand and help refine all the new processes and tasks. The software teams then set about creating and testing digital forms, workflows and record-keeping functions needed to bring those processes to life.

One result was Work Coordination & Control: a single, central system robust enough to receive, route and track all Facilities work requests, including those related to space management. The new system, based on IBM Maximo software, is currently handling up to 200 requests per day.

For space planners, another IT team worked with Tririga software to help build up the digital space inventory. The system now provides up-to-date space maps, with highly detailed descriptions of key features. Planners now can match these details to individual needs, and then place individuals and teams in more appropriate work spaces.

The team also saved significant time for Facilities workers by letting them manage large numbers of moves simultaneously, and automatically update many related records when a space changes hands. With roughly 3,000 moves each year, the new features are expected to save around \$30,000 annually.

Developers also provided a mobile solution that makes it easy for Facilities crews to record progress while in the field, instead of returning to the office to download or transfer data. Facilities personnel now rely on new or improved mobile capabilities for inventory management at the Facilities warehouse and simplified reporting of safety inspections.

Other key personnel for the changes included Mark Spoonamore, Mary Kay Hatfield, Maggie Sorensen, Steven Benner, Mike Muller, John Engelmann, Karen Henry, Colin Scroggins, Shauna Moore, Thomas Heisel, John Dykes and Peter Burton.

The work thus far marks only the first phase of planned changes. Carol Jones, chief information officer and director of IT Services, said her center looks forward to continuing the work.

"Our colleagues in Facilities are great partners," she said. "We're grateful for the chance to make work easier for them and their customers, and to increase efficiency at the Labs."



COORDINATING THE MOVING PARTS — Mary Watson, (left) manager of the Work Coordination and Control department, points out the different types of facilities area managers and their portfolios to Amy Moser, WCC tactical planner for projects/services coordination. The department determines how facilities work is executed and status is tracked. (Photo by Pam Patton)

Managing Sandia's unique facilities

By Jennifer Sawayda

When John Clymo became the associate labs director of Infrastructure Operations, he introduced a vision for revamping how Sandia manages buildings, space and infrastructure. That vision was based on years of experience. Before coming to the Labs, his career took him around the world to manage various military and government installations, as well as high-rise commercial facilities.

"There are a number of best practices I've seen in action and that I know Sandia can benefit from instituting when it comes to managing its facilities," John says.

Until recently, Sandia managed facilities in a decentralized manner. This created challenges for members of the workforce to know whom to contact with facilities-related concerns and for leadership to access comprehensive data that would help them make more informed investment decisions.

"Due to a variety of reasons, some quite valid, I think Sandia lost sight of how a professional property management organization can provide more strategic solutions to how we maintain and build our facilities to support our important mission work," John says.

Deployed approach

Mark Coffing is taking on one of the new roles as a facilities area manager (FAM). He will oversee a group of dedicated professionals who provide a range of services to residents of Technical Areas III and V.

"With this new deployed approach, we have more visibility with our building occupants and can more effectively address their needs," Mark says. The goal is to deliver more customized, more timely services. From a customer perspective, this should result in shorter response times for requests and improved status updates.

Using a customer service system based on industry best practices for property management will allow facilities personnel to track Sandia's assets while working in close partnership with the divisions, and the new facilities management system (FMS) will pull together the key support organizations necessary to operate and maintain buildings and other

spaces in a more agile manner.

The new system is organized into six areas managed by FAMs, and further divided into smaller areas called portfolios. Included are all Sandia properties at the New Mexico and California sites, leased buildings and remote facilities at the Kauai Test Facility in Hawaii, the Tonopah Test Range in Nevada and the Weapons Evaluation Test Laboratory in Texas.

Sharpening the 'FOCIS' on building needs

Rico Ortiz and Kimberly Pino are facilities area managers overseeing portfolios in Technical Area I. Prior to the new model, Rico and Kimberly were the only two operations managers for the entire New Mexico site.

Each of the six new managers will work with a team of facilities portfolio managers and others to meet the

unique facilities needs of each portfolio. To be closer to their customers, the teams will reside in dedicated Facilities Operations Customer Integration Space (FOCIS) rooms within each portfolio.

"We are providing a streamlined point of contact for customers," Kimberly says. "Customers can directly contact their building manager by visiting the FOCIS rooms or by calling the facilities help desk."

Eddie Garcia, building manager for the portfolio in Tech Area V, says this face-to-face collaboration with customers and the FAM teams will increase efficiency and quality.

"Our whole goal is to get better information so Facilities Maintenance can execute their work correctly the first time and in a timely manner," Eddie says. "This day-to-day collaboration will help us understand the tactical and strategic needs of our customers."

Mission Support control

The facilities management system requires a lockstep workflow between the Facilities and Emergency Management Center, which will interact with customers to determine needs and the scope of work, and Infrastructure Services, the center responsible for executing the work. A command-type center — the Work Coordination and Control department — will coordinate projects to determine how work is executed and communicate status.

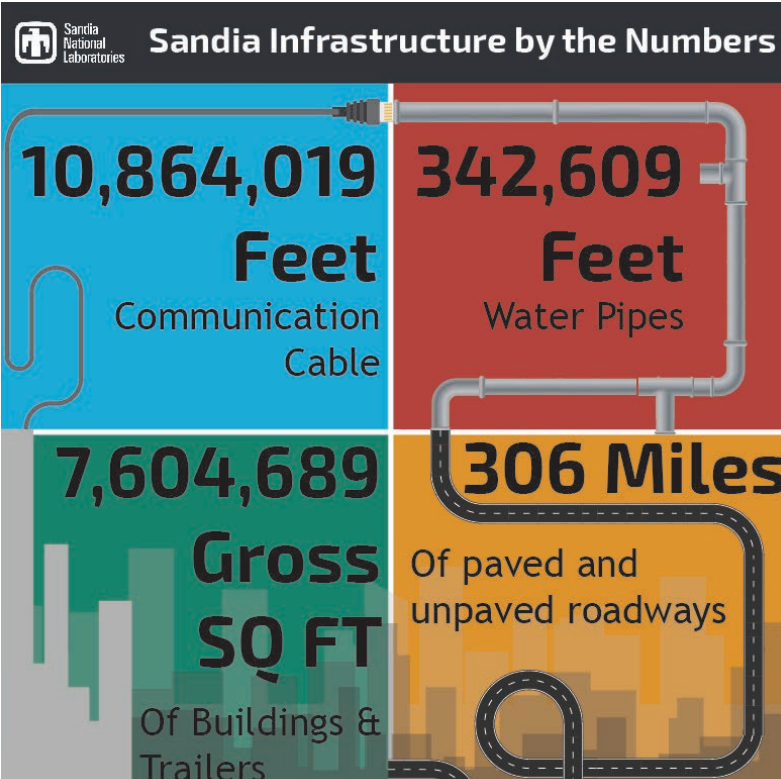
"This new work coordination component will help us better determine if the work truly meets customer expectations, or if corrections to the scope are needed," Mark explains. "With this integrated approach between groups, we should be able to identify maintenance issues more proactively and reduce the expense of emergency repairs."

The Infrastructure Engineering department also will take an active role at the beginning of the work control process.

"The building manager can go directly to engineering and problem solve," says Kimberly. "There will be less changing of hands under this new system, and engineering will be involved at the front end."


The implementation of the system will require a transition period in the facilities and infrastructure areas. However, John says he is confident this approach will build a solid structure to help set priorities for maintenance activities that sustain all the Labs facilities.

"Facilities management is a true art form," John says. "Everyone from our craft to our strategic site planners are committed to meeting the needs of our mission partners, and this new way of doing things will ensure Sandia's resources can respond to shifts in mission priorities."

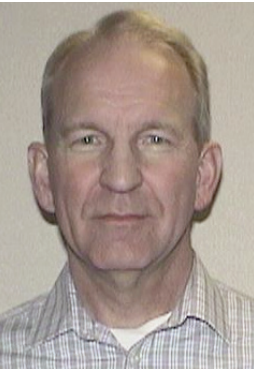


FAST FACILITIES FACTS (Infographic by Alicia Bustillos)

Mileposts



New Mexico photos by
Michelle Fleming
California photos by
Randy Wong



Brett Redmund 30



Kevin Eklund 35



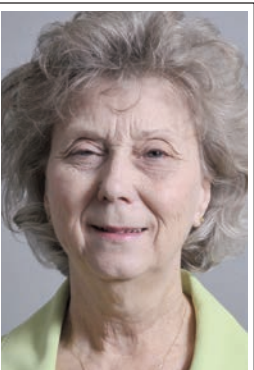
Sabine Boruff 30



Mark Howard 30

Recent Retirees





Delene Cox 25



Todd Bowling 25



Sidney Lee 25



Shanalyn Kemme 20



Lucille Forster 37



Lisa Garcia 30



Rebecca Lopez 20




Emily Wright 20



Bill Cowan 15



Christopher Duran 15



No photo available

Michael Hess 29



Howard Kimberly 30



Donna Gonzales 15



Jan Kohler 15



Bethany Martin 15



Leslie Phinney 15



Jens Schwarz 15



Clark Snow 15

Antibiotic pump

(Continued from page 1)

“The big breakthrough was in how we could take poor structural data from experiments and massage it to come up with an improved structure we could work with to understand the mechanism of the pump,” said Susan.

Molecular modeling reveals pump ‘lock’ and mechanism

Once they had the detailed structure of the pump, the real work began.

First, the team added a lipid membrane to model the real-world environment of the pump. Then, they ran computer simulations to see what the pump looks like with zero, one or two protons. Letting in two protons is the battery that powers this pump. They ran simulations to see the transition from the protein facing inside the bacterium to the outside to find the “easiest” path and thus see how the pump works. Modeling this “flip” took over 80,000 hours of computer processing.

They also ran simulations to see what the pump looks like with an example drug in the drug-binding pocket. Susan said they found lots of flexibility in the pocket where antibiotics would bind, which makes sense given that the pump can recognize a wide variety of drugs. They also identified a few critical amino acids that serve as a lock to make sure that the pump doesn’t let go of the protons willy-nilly.

“Antibiotic resistance is an important problem. The ‘lock’ on the pump is what makes this transporter tick. With this knowledge, in the future we can develop new antibiotics that aren’t pumped out or otherwise break the lock in EmrE,” said Vermaas. “If we figure out how to break the pump so it’s unregulated and leaks out protons, that would be a new way to kill bacteria.”

Additional research on countering antimicrobial resistance

In addition to her work on antibiotic pumps, Susan

has also modeled a protein that transports anthrax toxins into host cells where they wreak havoc, allowing the Bacillus anthracis bacteria to thrive and cause anthrax. Susan and her collaborators, including Sandia postdoc Mangesh Chaudhari, determined the molecular mechanisms of how these toxins make their way into the host cell and developed a plug to block this process. Sandia bioengineer Anson Hatch led a team that made and tested the plug.

In a three-year project also funded by Sandia’s Laboratory Research and Development program, Susan is studying a new antimicrobial called teixobactin. Teixobactin blocks the production of the bacterial cell wall in a unique way that is difficult for bacteria to develop resistance to. She and her collaborators from Sandia and Illinois are using computer simulations and experiments to understand how the antimicrobial functions to make it more potent and broad acting.

Though it’s challenging for gram-positive bacteria, such as staphylococcus aureus, to change how they make their cell wall to develop resistance to teixobactin, the antimicrobial can still be pumped out of bacteria before it does its damage, making Susan and Vermaas’ research to understand the mechanism of antibiotic pumps relevant.

Susan said, “Molecular dynamics modeling has very high resolution in space and time, which you don’t get from other experiments. We can see the dynamics over time in increments of one millionth of one billionth of a second. We can also see bits and pieces of a process that’s not resolved in experiments and determine which chemical structures contribute to the work involved. This gives us an advantage in learning how pathogens function, and that information can lead to new therapies to counter those pathogens.”

This project made extensive use of Sandia’s high-performance computing resources and was conducted at the Center for Integrated Nanotechnologies, a DOE Office of Science user facility jointly operated by Sandia and Los Alamos national laboratories.

Sandia’s LDRD office through the Campus Executive Program and the National Institutes of Health provided

funding for the research. The Defense Threat Reduction Agency’s Joint Science and Technology Office provided additional funding.

“The small investment from the Campus Executive Program was done after carefully reviewing dozens of proposal ideas before selecting this one on antibiotic pumps,” said Eric Ackerman, manager of the nanobiology department. “Josh visited Sandia to work directly with Susan and her team, and these direct interactions helped immensely. The project was also a lesson in perseverance; it took several years of work before the paper was published. Their paper demonstrates the power of modeling to massage low-resolution structural determinations into useful mechanistic understanding.”

Lab News rack locations

The Lab News is delivered to newspaper racks in the locations listed below every other Thursday afternoon.

Bldg. 802, elevator lobby	Bldg. 861, Cafeteria lobby
Bldg. 810, east lobby	Bldg. 870, lobby
Bldg. 822, south entrance	Bldg. 823, lobby
Bldg. 858 EL, lobby	Bldg. 701, next to elevator
Bldg. 880, Aisle D, north lobby	IPOC, lobby
Bldg. 892, lobby	CGSC, lobby
Bldg. 894, east entrance, lobby	CRSI, lobby
Bldg. 898, east lobby	M.O. 308, lobby
Bldg. 887, lobby	Bldg. 960, lobby
Bldg. 891, lobby	Bldg. 962 (TA III), lobby
Bldg. 836, lobby	Bldg. 6585 (TA V), lobby
Bldg. 831/832 north lobby	Bldg. 905, lobby
	800(A), outside of Vicki’s

SANDIA CLASSIFIED ADS

MISCELLANEOUS

SOUND SYSTEM, Bose, just like <https://tinyurl.com/y9qo4xx4>, \$70; metal file cabinets, 4-drawer, 3, \$75 ea. or \$200/all. Vigil, 575-386-6377.

CHICKERING & SONS PIANO, 1973, 1 owner, hardly used, excellent condition, \$1,200 OBO. Bennett, 505-299-1144.

DINING TABLE, w/4 chairs, dark cherry finish, good condition, few scratches, \$250 OBO. Hale, 405-229-4611.

KITCHEN TABLE, maple, 42-in. pedestal, w/3 leaves, 4 oak chairs, photo available, \$200. Walkington, 505-831-6974.

SOFA & LOVESEAT, DeCoro, Italian leather, w/4 recliners total, beautiful rust color, excellent condition, \$850. Hedrich, 505-220-8204.

ENTERTAINMENT CENTER, beautiful engraved wood, 3 pcs. total, call for photos, \$250 OBO. Gurule, 505-263-9935.

RUG, indoor, short pile, light tan, 18x 20, never used, \$20. Lewis, 505-323-7268.

DAYBED, Mahogany, w/XL twin mattress, real wood, new, unused mattress, paid >\$800, asking \$375. Brothers, 505-401-6140.

BALDWIN GRAND PIANO, 6'3", original owner, original price \$22,000, asking \$10,000. Sichler, 505-565-5885.

1914 PLAYER PIANO, vintage, Hamilton Manualo (Baldwin), w/39 word rolls, \$300. Burgett, 505-344-5945.

GOLF DRIVER, Taylor Made Rocketballz driver, 10.5 degree loft, adjustable, Sr. flex, used 6 rounds, \$100. Holmes, 505-873-5255.

SHOPSMITH MARK V, w/planer, jigsaw, sander, jointer, extension table, many other accessories, \$1,000. Judd, 505-250-8769.

STAND MIXER, KitchenAid, bowl-lift, 4-1/2 qt. stainless bowl, flat beater, dough hook, w/instructions, 350-W, \$75. Hatch, 505-221-4477.

TRANSPORTATION

'07 FORD F150, supercab, 8-cyl., 5.4 Triton, 1 owner, looks and runs great, <37K miles, \$14,000. Jones, 505-235-5110.

'51 CHEVROLET DELUXE, 4-dr., original paint, new upholstery, great condition, \$12,500. Owens, 505-980-6796, ask for Norman.

'00 TOYOTA CELICA, AT, updated by mechanic, 168K miles, great condition inside & out, \$3,800 OBO. Ellis, 505-459-8542.

'13 MAZDA CX-5, AWD, touring, navigation, roof rack, only 22K miles, excellent condition, KBB \$18,000, asking \$16,500 OBO. Martin, 623-687-7673.

'14 FORD F150, single cab, 4x2, EcoBoost, black, black rims, camera, Bluetooth, 73K miles, \$23,500. Ahr, 505-315-8584.

'15 MERCEDES SLK 250, Indium gray w/beige interior, 22K miles, excellent condition, \$31,000 OBO. Somuk, 505-377-5900, msomuk@yahoo.com.

'11 BMW 328i, AT, 4-dr., w/sports & winter pkg., 41K miles, great condition, \$13,000. Sokolowski, 505-615-8618.

'01 CHEVY SILVERADO 2500 HD, crew cab, tow pkg., 105K miles, 1 owner, new tires, KBB \$8,400. Bentley, 505-331-5788.

'05 FORD F350 SRW, 6.0L, service records, keyless entry, camper & tow pkgs., torklift bumpers & superhitch, 66K miles, \$16,500. Burr, 575-854-3434.

'79 CORVETTE, w/AC, PW, T-tops, PL, second owner, 26K miles, \$22,000 OBO. Montoya, 505-507-7980.

RECREATION

'06 SUZUKI DRZ400SM, many upgrades/extras, including Enduro & SM wheel sets, 16K miles, \$5,000. Mitchell, 505-850-7307.

How to submit classified ads

- EMAIL: Michelle Fleming (classads@sandia.gov)
- FAX: 505-844-0645
- MAIL: MS 1468 (Dept. 3651)
- INTERNAL WEB: From Techweb, search for 'NewsCenter.' At the bottom of that page, click the 'Submit an article' button. Due to space constraints, ads will be printed on a first-come basis.

DEADLINE: Friday noon before week of publication unless changed by holiday.

Questions to Michelle Fleming at 505-844-4902.

STARCRAFT TRUCK POP-UP CAMPER, heater, refrigerator, gas or electric, AC, gas cook top, fits 7-ft. truck bed, \$3,599. Hibray, 505-821-3455.

REAL ESTATE

3.5 ACRES, north of Edgewood, off Hwy. 344, Entranosa water & electricity readily available, wooded, beautiful vistas, county road access, \$40,000. Hatch, 505-221-4477.

4-BDR. HOME, 2-1/2 baths, 2,555-sq. ft., NE Heights, North Star Elementary, La Cueva High, \$399,000. Chavez, 720-339-3544.

4-BDR. HOME, Hidden Valley, near Four Hills, beautifully remodeled, Zillow.com: 713 Fennel Ct. SE, neighborhood pool, \$259,900. Volker-Rector, 505-710-6290.

WANTED

BEDROOM FURNITURE, good condition, queen or king bed, w/matching nightstands & dresser. Rhea, 505-227-4799.

CAT/HOUSE SITTER, responsible, Sept. 27-Oct. 2, must have experience & excellent references. Ward, 505-292-1618.

MINIVAN, good condition, preferably white, Asian make, <\$10,000. Appel, 505-750-8419.

FOREVER HOME, action-oriented, neutered, black lab, 5 yrs. old, former companion to elderly lady. Lauben, 505-980-2915.

SMALL PICKUP, good condition, AC. Lucero, 505-440-9893.

Ad rules

1. Limit 18 words, including last name and home phone (If you include a web or e-mail address, it will count as two or three words, depending on length of the address.)
2. Include organization and full name with the ad submission.
3. Submit ad in writing. No phone-ins.
4. Type or print ad legibly; use accepted abbreviations.
5. One ad per issue.
6. We will not run the same ad more than twice.
7. No "for rent" ads except for employees on temporary assignment.
8. No commercial ads.
9. For active Sandia members of the workforce, retired Sandians, and DOE employees.
10. Housing listed for sale is available without regard to race, creed, color, or national origin.
11. Work Wanted ads limited to student-aged children of employees.
12. We reserve the right not to publish any ad that may be considered offensive or in poor taste.

70%

of APS students qualify for free or reduced school meals.

58,000 students in APS live at or below \$44,000 a year per household of four.

74%

of APS schools are identified Title I eligible.

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As many as

5,000

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July 23–August 6, 2018

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Ask your OAA about drop off locations in your area. For a list of supply needs or to give online, visit community.sandia.gov

Employee death: Student intern Gregory Brunson

Gregory Brunson, a student intern, had a great impact on the work of Sandia's robotics research program during his four years working at Sandia, his manager said.

Gregory died June 10.

"From the day he started working while still in high school and throughout the years he worked with us, Greg demonstrated a positive, can-do attitude and consistently added an innovative element to the teams and projects he supported while here," said his manager, Jon Salton.

Greg was hired by the robotics group in May 2014.

"His intellect, pleasant smile and bright personality will be sorely missed by everyone he touched," Jon said.



Student intern Gregory Brunson died on June 10.

(Photo courtesy of Sandia National Laboratories)

First responders confront shooters, explosives in emergency exercise



Photos by Randy Montoya



More than 200 members of Sandia’s workforce got a realistic taste of what might happen in a shooting incident on July 25 in the annual full-scale emergency exercise at the New Mexico site.

The scenario began as a multiple casualty, active shooter incident. First responders, including Sandia protective force officers and emergency response personnel, were first on the scene, working to control the incident in Tech Area V, secure buildings, and triage and treat the wounded.

The incident quickly evolved into a hostage situation. Security forces and emergency responders from the 377th Air Base Wing, the FBI, NNSA and the Albuquerque Police Department provided additional support. The Kirtland Air Force Base and Bernalillo County fire departments and Albuquerque Fire Rescue crews, along with Albuquerque Ambulance Service, transported patients to area hospitals.

During the hours-long standoff, an Air Force K-9 identified explosives in a shooter’s vehicle, prompting responders to call for a Kirtland explosive ordnance disposal team to disarm the device.

Emergency Management uses the annual exercise to verify the effectiveness of its program and evaluate how well the program and responders follow the site’s plans and procedures and the Department of Energy order covering the comprehensive emergency management system.

— Lindsey Kibler



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